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A multigrid finite element solver for the Cahn–Hilliard equation

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Abstract

A multigrid finite element solver for the Cahn–Hilliard equation is presented that has mesh-independent convergence rates for any time-step size, including in the important limit $\epsilon \to 0$ which is examined via numerical examples. Numerics are performed for a number of test problems which show that the features of the Cahn–Hilliard equation (minimising interface measure, Lyapunov energy functional etc.) are preserved. We also explore the use of this solver in conjunction with adaptive time-stepping and adaptive mesh strategies.

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1. Introduction

The Cahn–Hilliard equation [6,7] was originally introduced as a phenomenological model of phase separation in a binary alloy. More recently, it has been used to study phase transitions and interface dynamics, related free boundary problems, multiphase fluids and polymer solutions, see [5,17,21] and the references therein.

The equation, together with appropriate initial and boundary conditions,

$$\frac{\partial c}{\partial t} - \nabla \cdot (B(c)\nabla w) = 0, \tag{1a}$$

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$$w - \frac{1}{\epsilon}\Phi'(c) + \epsilon\Delta c = 0 \qquad \text{in } \Omega_T := \Omega \times (0,T), \tag{1b}$$

$$\frac{\partial c}{\partial \hat{n}} = B\frac{\partial w}{\partial \hat{n}} = 0 \qquad \text{on } \partial\Omega_T := \partial\Omega \times (0,T), \tag{1c}$$

$$c(\mathbf{x},0) = c_0(\mathbf{x}), \tag{1d}$$

where $\Omega \subset \mathbb{R}^d (d = 1,\ldots,3)$ is a bounded polygonal domain and $\hat{n}$ is the outward pointing unit normal to Ω, form (in effect) a fourth order non-linear parabolic partial differential equation. The parameter ϵ is a measure of the interfacial thickness and Φ is a double well potential with its global minima at $c = \pm 1$, typically

$$\Phi(c) = \frac{1}{4}(1-c^2)^2. \tag{2}$$

For derivation and analysis of the equation we refer to [12,13,10,15] and the references therein. The mobility function $B(c)$ is often taken to be constant ($B \equiv 1$). Here, we consider this choice as well as the thermodynamically reasonable choice [8]

$$B(c) = [1-c^2]_+ := \max\{0, 1-c^2\}. \tag{3}$$

It is well known that the Cahn–Hilliard equation is a gradient flow of the Lyapunov energy functional:

$$J(c) = \int_\Omega \frac{1}{\epsilon}\Phi(c) + \frac{\epsilon}{2}|\nabla c|^2 \,\mathrm{d}\mathbf{x}, \tag{4}$$

which is therefore non-increasing in time, we wish this to carry over to a discrete version of this functional in our numerical scheme.

Numerical simulations of the Cahn–Hilliard equation are difficult on a normal computer in a reasonable time because fourth order non-linear equations impose severe time-step restrictions on explicit methods ($\tau \sim h^4$) so implicit methods must be used. Additionally in order to fully capture the interface dynamics high spatial resolution is required, typically at least 8–10 elements (see [14], if there are an insufficient number of elements spurious numerical solutions can be introduced). In complicated problems that require uniform refinement this leads to large algebraic problems to be solved at each time-step.

The interface profile is given by (see for example [11])

$$\tanh\left(\frac{1}{\epsilon\sqrt{2}}x\right). \tag{5}$$

Thus, if we consider the interfacial region to be where the concentration c varies between -0.99 and 0.99 a simple calculation yields that the interface has its width given by width $\approx 7.5\epsilon$ (we note that this is more than twice as large as the interface for the "double-obstacle" free energy [4] which has width $\pi\epsilon$).

Traditionally iterative solution methods such as Gauss–Seidel have been used (for example [10]) but these suffer from slow convergence rates, typically O(N), where N is the number of points in the discretisation. Each iteration of a Gauss–Seidel solver is an O(N) operation and under a suitable choice of semi-implicit temporal discretisation (see below) there are no time-step restrictions. This makes the total work required for the Gauss–Seidel method O(N^2). A non-linear multigrid method for a finite difference approximation of this problem has recently been suggested by Kim et al. [17,18] which exhibits convergence rates independent of N as long as a weak time-step restriction related to the initial data is observed. The method presented here is an extension of that of Kornhuber and Krause [20] which has convergence rates independent of N with no time-step restriction. Each iteration of this multigrid solver is an O(N) operation, making the total work required O(N).